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Three-Dimensional Cartesian
Particle-in-Cell Calculations

by

William R. Gage
Charles L. Mader

ABSTRACT

A study of the Particle-In-Cell method of numerically solving hydrodynamic problems in three dimensions is described. The closure of a cubical void in a cubical box was successfully computed. Various methods, including stereoscopic views, of pictorial description of the particle positions are described.

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CONTENTS

FIGURES

I. INTRODUCTION

The Particle-In-Cell method[1] for numerically solving two-dimensional hydrodynamic problems with chemical reaction and realistic equations of state has been remarkably successful in describing the formation of hot spots when shocks interact with density discontinuities[2,3]. The Particle-In-Cell method allows large distortions to occur in the fluid and permits void closure. Because of these unique characteristics, the Particle-In-Cell method is the obvious one to use to solve the three-dimensional problem of shocks interacting with many voids. While sufficiently fast computers to resolve such a problem in detail will not be available for several years, we have investigated the Particle-In-Cell method in three dimensions to determine if the techniques used in the two-dimensional EIC code[2,3] were adequate when extended to three dimensions. The results presented in this report show that the Particle-In-Cell method is adequate.

II. COMPUTATIONAL METHOD

The calculational technique used is the PIC (Particle-In-Cell) scheme described in detail in Appendix A.

The equation of state used to describe the fluid is the HOM equation of state for nitromethane described in reference 2.

The calculations were performed using an IBM 7030 (STRETCH) code written as part of this study.

Accuracy in resolving the dynamics is dependent upon the number of cells and particles. For practical purposes, the accuracy is limited by the amount of machine time that is available. In the calculations reported here, 1728 cells were used with 12 cells in each of the X, Y, Z directions. We used 16 particles per cell, or a total of 27,648 particles. Such a crude mesh is adequate for studying the method, but would not give sufficient resolution for most problems of interest.

III. VOID CLOSURE

The model studied was a cube of nitromethane with 12 cells on a side containing a cubical void with 4 cells on a side. The model is shown in Figure 1 with the coordinate system which was used. A piston is applied to the bottom of the cube, shocking the nitromethane to 85 kbar.

We also studied the reactive flow problem of a 125-kbar shock driving a detonation through the cube of nitromethane. The results compared well with those obtained in one and two dimensions.

The particle positions of each of the 12 layers of cells in the Z direction are shown in Figure 2.

The particle positions of each of 16 equally spaced layers through the void in the Z direction are shown in Figure 3.

Stereo projections of half the cells and all the cells through the void are shown in Figures 4 and 5. With a viewer, a stereo effect is achieved. The angle of observation and particular amount of information to be displayed depends upon the problem; however, stereo projections are a useful method of presentation of the results, and the method is described in Appendix B.

Perhaps the most useful method of presenting the results is to make clear prints of the 24 layers of particles in half of the cube and mount them to scale in grooved Lucite boxes. By this technique, one obtains a three-dimensional scale model.

IV. CONCLUSIONS

The Particle-In-Cell method has been successfully extended to three dimensions. Various methods of pictorial description of the results were tried. Each method had its uses, with the three-dimensional model being the most informative, but least convenient. Solution of three-dimensional hydrodynamic problems of practical interest appears to be possible as soon as computers with sufficient speed (at least 100 times faster than STRETCH) are available.
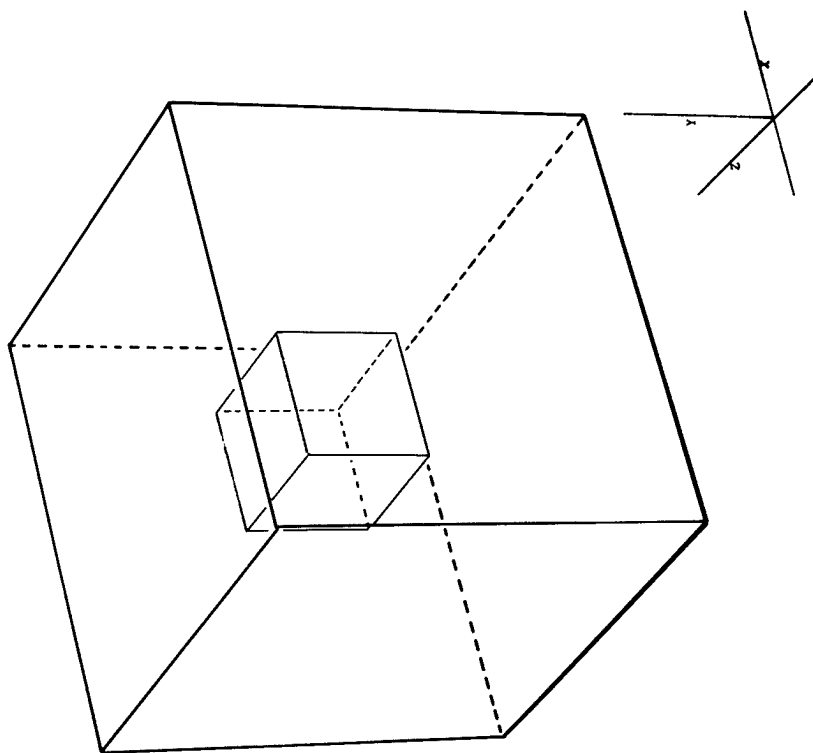
Fig. 1. A cube of nitromethane containing a centered cubical void.

Figure 2

The particle positions at various times for a cube of nitro-methane, 0.024 cm on a side, containing a cubical void 0.008 cm on a side. The 0.024-cm side in the Z direction of the cube is cut into 12 equally spaced layers. A piston is applied to the bottom of the cube. Each group of 12 pictures presents views of the layers in succession as seen looking through the x,y face of the cube.

Figure 3

The particle positions at various times for a cube of nitromethane containing a cubical void cut into 16 equally spaced layers in the Z direction. Each group of 16 pictures presents views of the successive layers through the void.

Figure 4

The particle positions through half of the void shown at various times in stereo projections looking down into the void at a 15° angle.

Figure 5

The particle positions through all of the void shown at various times in stereo projections looking down into the void at a 15° angle.

APPENDIX A

THE HYDRODYNAMIC EQUATIONS

The Particle-In-Cell method of Harlow[1] has been used by Mader[2,3] to solve reactive two-dimensional fluid flow problems. We shall present a description of the equations used to solve the three-dimensional fluid flow problem. The equations are a straightforward extension of the PIC equations described by Mader[2].

The three-dimensional partial differential equations for nonviscous, nonconducting, compressible fluid flow are:

$$\frac{\partial \rho}{\partial t} + U_x\left(\frac{\partial \rho}{\partial x}\right) + U_y\left(\frac{\partial \rho}{\partial y}\right) + U_z\left(\frac{\partial \rho}{\partial z}\right) = -\rho\left(\frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}\right)$$

$$\rho\left[\frac{\partial U_x}{\partial t} + U_x\left(\frac{\partial U_x}{\partial x}\right) + U_y\left(\frac{\partial U_x}{\partial y}\right) + U_z\left(\frac{\partial U_x}{\partial z}\right)\right] = -\frac{\partial P}{\partial x}$$

$$\rho\left[\frac{\partial U_y}{\partial t} + U_x\left(\frac{\partial U_y}{\partial x}\right) + U_y\left(\frac{\partial U_y}{\partial y}\right) + U_z\left(\frac{\partial U_y}{\partial z}\right)\right] = -\frac{\partial P}{\partial y}$$

$$\rho\left[\frac{\partial U_z}{\partial t} + U_x\left(\frac{\partial U_z}{\partial x}\right) + U_y\left(\frac{\partial U_z}{\partial y}\right) + U_z\left(\frac{\partial U_z}{\partial z}\right)\right] = -\frac{\partial P}{\partial z}$$

$$\rho\left[\frac{\partial I}{\partial t} + U_x\left(\frac{\partial I}{\partial x}\right) + U_y\left(\frac{\partial I}{\partial y}\right) + U_z\left(\frac{\partial I}{\partial z}\right)\right] = -P\left(\frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}\right).$$

In the PIC method, the dynamic quantities of the fluid are associated with a fixed (Eulerian) mesh of cells, and the fluid itself is represented by a set of mass points or particles resident in the cells. The conservation of mass is automatically satisfied by the particle model. Since the particles are not moved in Phase I, the transport terms in the momentum and energy equations may be dropped, resulting in the following set of equations:

Momentum

$$\rho \frac{\partial U_x}{\partial t} = - \frac{\partial P}{\partial x}$$

$$\rho \frac{\partial U_y}{\partial t} = - \frac{\partial P}{\partial y}$$

$$\rho \frac{\partial U_z}{\partial t} = - \frac{\partial P}{\partial z}$$

Energy

$$\rho \frac{\partial I}{\partial t} = - P\left(\frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}\right)$$

With artificial viscosity these equations become:

$$\rho \frac{\partial U_x}{\partial t} = - \frac{\partial (P + Q)}{\partial x}$$

$$\rho \frac{\partial U_y}{\partial t} = - \frac{\partial (P + Q)}{\partial y}$$

$$\rho \frac{\partial U_z}{\partial t} = - \frac{\partial (P + Q)}{\partial z}$$

$$-\rho \frac{\partial I}{\partial t} = P\left[\frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}\right] +$$

$$+ \frac{\partial (U_x Q)}{\partial x} - U_x \frac{\partial Q}{\partial x} + \frac{\partial (U_y Q)}{\partial y} - U_y \frac{\partial Q}{\partial y}$$

$$+ \frac{\partial (U_z Q)}{\partial z} - U_z \frac{\partial Q}{\partial z} .$$

Given some initial conditions, these equations are solved using finite-difference approximations.

Each cycle advancement is performed in three phases. In Phase I the cell quantities are updated using the above differential equations. In Phase II the particles are moved carrying with them the appropriate fractions of mass, momentum, and energy. Finally, in Phase III the amount of chemical reaction is calculated and the pressure and temperature of each cell are calculated using the HOM equation of state.

The problem is set up with a cubical lattice of 1728 cells (12 in each direction). Every cell has three indices (i,j,k) associated with it, each index having a range from zero to eleven. The (x, y, z) coordinates of the corner nearest the origin of cell i,j,k are then (iS, jS, kS) where S is the length of the side of a cell. The faces of each cell are numbered one through six.

The faces of cell i,j,k have indices

face 1   i, j - 1/2, k
face 2   i + 1/2, j, k
face 3   i, j + 1/2, k
face 4   i - 1/2, j, k

face 5   i, j, k + 1/2

face 6   i, j, k - 1/2 .

The particles are initially arranged in the same pattern in all cells. Their coordinates are such that no two particles in a cell have the same x, y, or z coordinates. For example, in cell i = 0, j = 0, k = 0, with unit side length, the sixteen particles have the following coordinates.

$(\frac{1}{17}, \frac{4}{17}, \frac{1}{17})$ $(\frac{5}{17}, \frac{3}{17}, \frac{27}{34})$ $(\frac{9}{17}, \frac{2}{17}, \frac{19}{38})$ $(\frac{13}{17}, \frac{1}{17}, \frac{35}{38})$

$(\frac{2}{17}, \frac{8}{17}, \frac{21}{34})$ $(\frac{6}{17}, \frac{7}{17}, \frac{6}{17})$ $(\frac{10}{17}, \frac{6}{17}, \frac{57}{38})$ $(\frac{14}{17}, \frac{5}{17}, \frac{5}{38})$

$(\frac{3}{17}, \frac{12}{17}, \frac{3}{17})$ $(\frac{7}{17}, \frac{11}{17}, \frac{31}{34})$ $(\frac{11}{17}, \frac{10}{17}, \frac{27}{38})$ $(\frac{15}{17}, \frac{9}{17}, \frac{41}{38})$

$(\frac{4}{17}, \frac{16}{17}, \frac{25}{34})$ $(\frac{8}{17}, \frac{15}{17}, \frac{8}{17})$ $(\frac{12}{17}, \frac{14}{17}, \frac{5}{38})$ $(\frac{16}{17}, \frac{13}{17}, \frac{13}{38})$

To begin the problem, the cell quantities (mass, velocities, pressure, temperature, internal energy, and mass fraction) are set to initial values and the particle mass is set to 1/16 of the mass of its resident cell.

Phase I is not performed for empty cells nor for piston boundary cells.

A. Calculate the pressures on the six faces of each cell.

1. If a cell face is on a boundary, its pressure is set equal to the cell pressure.

2. If a neighbor cell is empty, the pressure on that face is set to zero.

3. Otherwise:

$P^1_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i,j-1,k}\right)$ face 1 of cell ijk

$P^2_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i+1,j,k}\right)$ face 2 of cell ijk

$P^3_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i,j+1,k}\right)$ face 3 of cell ijk

$P^4_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i-1,j,k}\right)$ face 4 of cell ijk

$P^5_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i,j,k+1}\right)$ face 5 of cell ijk

$P^6_{i,j,k} = \frac{1}{2}\left(P_{i,j,k} + P_{i,j,k-1}\right)$ face 6 of cell ijk.

B. Calculate the viscosities on the six faces of each cell.

1. If a neighbor cell is empty, the viscosity on that face is set to zero.

2. If the viscosity is negative, it is set to zero.

3. If a cell face is on a boundary, its viscosity is set to zero.

4. For the problems run on the 12 x 12 x 12 cell lattice, K = 1 was sufficient. It may be necessary to go to higher or variable K's in problems of greater resolution.

$$\bar{U}^4_{x,i,j,k} = \frac{1}{4}\left(\bar{U}_{x,i,j,k} + U_{x,i,j,k} + U_{x,i-1,j,k} + \bar{U}_{x,i-1,j,k}\right)$$

$$\bar{U}^2_{x,i,j,k} = \frac{1}{4}\left(\bar{U}_{x,i,j,k} + U_{x,i,j,k} + U_{x,i+1,j,k} + \bar{U}_{x,i+1,j,k}\right)$$

$$\bar{U}^1_{y,i,j,k} = \frac{1}{4}\left(\bar{U}_{y,i,j,k} + U_{y,i,j,k} + U_{y,i,j-1,k} + \bar{U}_{y,i,j-1,k}\right)$$

$$\bar{U}^3_{y,i,j,k} = \frac{1}{4}\left(\bar{U}_{y,i,j,k} + U_{y,i,j,k} + U_{y,i,j+1,k} + \bar{U}_{y,i,j+1,k}\right)$$

$$\bar{U}^5_{z,i,j,k} = \frac{1}{4}\left(\bar{U}_{z,i,j,k} + U_{z,i,j,k} + U_{z,i,j,k-1} + \bar{U}_{z,i,j,k-1}\right)$$

$$\bar{U}^5_{z,i,j,k} = \frac{1}{4}\left(\bar{U}_{z,i,j,k} + U_{z,i,j,k} + U_{z,i,j,k+1} + \bar{U}_{z,i,j,k+1}\right)$$

2. The tentative cell energy is then

$$\bar{I}_{i,j,k} = I_{i,j,k} + \frac{\Delta t\, S^2}{M_{i,j,k}} \left\{ P_{i,j,k}\left(U^4_{x,i,j,k} - U^2_{z,i,j,k}\right)\right.$$

$$+ U^1_{y,i,j,k} - U^3_{y,i,j,k} + U^6_{z,i,j,k} - U^5_{z,i,j,k}$$

$$+ q^4_{i,j,k}\, U^4_{x,i,j,k} - q^2_{i,j,k}\, U^2_{x,i,j,k}$$

$$+ q^1_{i,j,k}\, U^1_{y,i,j,k} - q^3_{i,j,k}\, U^3_{y,i,j,k} + q^6_{i,j,k}\, U^6_{z,i,j,k}$$

$$\left. - q^5_{i,j,k}\, U^5_{z,i,j,k}\right\}$$

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$$q^1_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i,j-1,k}}{2\left(M_{i,j,k} + M_{i,j-1,k}\right)}\left(\frac{U_{y,i,j-1,k} - U_{y,i,j,k}}{S}\right)^3$$

$$q^2_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i+1,j,k}}{2\left(M_{i,j,k} + M_{i+1,j,k}\right)}\left(\frac{U_{x,i,j,k} - U_{x,i+1,j,k}}{S}\right)^3$$

$$q^3_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i,j+1,k}}{2\left(M_{i,j,k} + M_{i,j+1,k}\right)}\left(\frac{U_{y,i,j,k} - U_{y,i,j+1,k}}{S}\right)^3$$

$$q^4_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i-1,j,k}}{2\left(M_{i,j,k} + M_{i-1,j,k}\right)}\left(\frac{U_{x,i-1,j,k} - U_{x,i,j,k}}{S}\right)^3$$

$$q^5_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i,j,k+1}}{2\left(M_{i,j,k} + M_{i,j,k+1}\right)}\left(\frac{U_{z,i,j,k} - U_{z,i,j,k+1}}{S}\right)^3$$

$$q^6_{i,j,k} = \frac{K\, M_{i,j,k}\, M_{i,j,k-1}}{2\left(M_{i,j,k} + M_{i,j,k-1}\right)}\left(\frac{U_{z,i,j,k-1} - U_{z,i,j,k}}{S}\right)^3$$

C. Tentative velocities are calculated according to the momentum equations above.

$$\bar{U}_{x,i,j,k} = U_{x,i,j,k} + \frac{\Delta t\, S^2}{M_{i,j,k}}\left(P^4_{i,j,k} - P^2_{i,j,k} + q^4_{i,j,k} - q^2_{i,j,k}\right)$$

$$\bar{U}_{y,i,j,k} = U_{y,i,j,k} + \frac{\Delta t\, S^2}{M_{i,j,k}}\left(P^1_{i,j,k} - P^3_{i,j,k} + q^1_{i,j,k} - q^3_{i,j,k}\right)$$

$$\bar{U}_{z,i,j,k} = U_{z,i,j,k} + \frac{\Delta t\, S^2}{M_{i,j,k}}\left(P^6_{i,j,k} - P^5_{i,j,k} + q^6_{i,j,k} - q^5_{i,j,k}\right)$$

D. Calculate tentative cell internal energies.

1. Calculate tentative velocity averages. If a neighbor cell is empty, the average velocity for that face is $\frac{1}{2}\left(\bar{U}_{i,j,k} + U_{i,j,k}\right)$.

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E. Calculate total cell energy and momenta.

$$\bar{E}_{i,j,k} = M_{i,j,k}\left[\bar{I}_{i,j,k} + \frac{1}{2}\left(\bar{U}^2_{x,i,j,k} + \bar{U}^2_{y,i,j,k} + \bar{U}^2_{z,i,j,k}\right)\right]$$

$$\bar{X}_{x,i,j,k} = M_{i,j,k}\,\bar{U}_{x,i,j,k}$$
$$\bar{X}_{y,i,j,k} = M_{i,j,k}\,\bar{U}_{y,i,j,k}$$
$$\bar{X}_{z,i,j,k} = M_{i,j,k}\,\bar{U}_{z,i,j,k}$$

PHASE II

For the movement of the particles, the velocity is determined by a method of weighting. A cube, the size of a cell, is imagined with the particle at its center. In general, this cube intersects eight cells with a certain fraction of its volume in each. The tentative velocities of the overlapped cells, weighted by their respective fractions of the volume, are added together to form the particle velocity. Those parts of the cube that fall outside the boundaries or intersect an empty cell are not used in the weighting.

The position of the particles in the cell determines which neighboring cells are used in the weighting. For a particle with coordinates (x, y, z) residing in cell ijk (i.e., $i \le x/S \le i+1$; $j \le y/S \le j+1$; and $k \le z/S \le k+1$) the eight different cases are:

1. $i \le x/S \le i+1/2$
   $j \le y/S \le j+1/2$
   $k \le z/S \le k+1/2$

2. $i \le x/S \le i+1/2$
   $j+1/2 \le y/S \le j+1$
   $k \le z/S \le k+1/2$

3. $i \le x/S \le i+1/2$
   $j+1/2 \le y/S \le j+1$
   $k+1/2 \le z/S \le k+1$

4. $i \le x/S \le i+1/2$
   $j \le y/S \le j+1/2$
   $k+1/2 \le z/S \le k+1$

5. $i+1/2 \le x/S \le i+1$
   $j \le y/S \le j+1/2$
   $k \le z/S \le k+1/2$

6. $i+1/2 \le x/S \le i+1$
   $j \le y/S \le j+1/2$
   $k+1/2 \le z/S \le k+1/2$

7. $i+1/2 \le x/S \le i+1$
   $j+1/2 \le y/S \le j+1$
   $k+1/2 \le z/S \le k+1$

8. $i+1/2 \le x/S \le i+1$
   $j \le y/S \le j+1/2$
   $k+1/2 \le z/S \le k+1$

The weighted particle velocities for each of these cases are as follows [(x, y, z) the coordinates of the particle in cell ijk with no faces on a boundary].

1. $V_1 = (iS + S/2 - x)(jS + S/2 - y)(kS + S/2 - z)$
   $V_2 = (iS + S/2 - x)(y + S/2 - jS)(kS + S/2 - z)$
   $V_3 = (iS + S/2 - x)(y + S/2 - jS)(z + S/2 - kS)$
   $V_4 = (iS + S/2 - x)(jS + S/2 - y)(z + S/2 - kS)$
   $V_5 = (x + S/2 - iS)(jS + S/2 - y)(kS + S/2 - z)$
   $V_6 = (x + S/2 - iS)(y + S/2 - jS)(kS + S/2 - z)$
   $V_7 = (x + S/2 - iS)(y + S/2 - jS)(z + S/2 - kS)$
   $V_8 = (x + S/2 - iS)(jS + S/2 - y)(z + S/2 - kS)$

$$\vec{U}_x = \left(V_1 \bar{U}_{x,i-1,j-1,k-1} + V_2 \bar{U}_{x,i-1,j,k-1} + V_3 \bar{U}_{x,i-1,j,k} + V_4 \bar{U}_{x,i-1,j-1,k} + V_5 \bar{U}_{x,i,j-1,k-1} + V_6 \bar{U}_{x,i,j,k-1} + V_7 \bar{U}_{x,i,j,k} + V_8 \bar{U}_{x,i,j-1,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5 + V_6 + V_7 + V_8\right)$$

$$\vec{U}_y = \left(V_1 \bar{U}_{y,i-1,j-1,k-1} + V_2 \bar{U}_{y,i-1,j,k-1} + V_3 \bar{U}_{y,i-1,j,k} + V_4 \bar{U}_{y,i-1,j-1,k} + V_5 \bar{U}_{y,i,j-1,k-1} + V_6 \bar{U}_{y,i,j,k-1} + V_7 \bar{U}_{y,i,j,k} + V_8 \bar{U}_{y,i,j-1,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5 + V_6 + V_7 + V_8\right)$$

$$U_z^1 = \left(V_1 \, \bar{U}_{z,i-1,j,k-1} + V_2 \, \bar{U}_{z,i-1,j+1,k-1} + V_3 \, \bar{U}_{z,i-1,j+1,k}\right.$$
$$+ V_4 \, \bar{U}_{z,i-1,j,k-1} + V_5 \, \bar{U}_{z,i,j,k-1} + V_6 \, \bar{U}_{z,i,j+1,k-1}$$
$$\left. + V_7 \, \bar{U}_{z,i,j+1,k} + V_8 \, \bar{U}_{z,i,j,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5 + V_6\right.$$
$$\left. + V_7 + V_8\right)$$

3.
$V_1 = (iS + S/2 - x)(jS + 3S/2 - y)(kS + 3S/2 - z)$
$V_2 = (iS + S/2 - x)(y - S/2 - jS)(kS + 3S/2 - z)$
$V_3 = (iS + S/2 - x)(y - S/2 - jS)(z - S/2 - kS)$
$V_4 = (iS + S/2 - x)(jS + 3S/2 - y)(z - S/2 - kS)$
$V_5 = (x + S/2 - iS)(jS + 3S/2 - y)(kS + 3S/2 - z)$
$V_6 = (x + S/2 - iS)(y - S/2 - jS)(kS + 3S/2 - z)$
$V_7 = (x + S/2 - iS)(y - S/2 - jS)(z - S/2 - kS)$
$V_8 = (x + S/2 - iS)(jS + 3S/2 - y)(z - S/2 - kS)$

$$U_x^1 = \left(V_1 \, \bar{U}_{x,i-1,j,k} + V_2 \, \bar{U}_{x,i-1,j+1,k} + V_3 \, \bar{U}_{x,i-1,j+1,k}\right.$$
$$+ V_4 \, \bar{U}_{x,i-1,j,k+1} + V_5 \, \bar{U}_{x,i,j,k} + V_6 \, \bar{U}_{x,i,j+1,k}$$
$$\left. + V_7 \, \bar{U}_{x,i,j+1,k+1} + V_8 \, \bar{U}_{x,i,j,k+1}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5\right.$$
$$\left. + V_6 + V_7 + V_8\right)$$

$$U_y^1 = \left(V_1 \, \bar{U}_{y,i-1,j,k} + V_2 \, \bar{U}_{y,i-1,j+1,k} + V_3 \, \bar{U}_{y,i-1,j+1,k}\right.$$
$$+ V_4 \, \bar{U}_{y,i-1,j,k+1} + V_5 \, \bar{U}_{y,i,j,k} + V_6 \, \bar{U}_{y,i,j+1,k-1}$$
$$\left. + V_7 \, \bar{U}_{y,i,j+1,k+1} + V_8 \, \bar{U}_{y,i,j,k+1}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5\right.$$
$$\left. + V_6 + V_7 + V_8\right)$$

$$U_z^1 = \left(V_1 \, \bar{U}_{z,i-1,j-1,k-1} + V_2 \, \bar{U}_{z,i-1,j,k-1} + V_3 \, \bar{U}_{z,i-1,j,k}\right.$$
$$+ V_4 \, \bar{U}_{z,i-1,j-1,k} + V_5 \, \bar{U}_{z,i,j,k-1} + V_6 \, \bar{U}_{z,i,j,k-1}$$
$$\left. + V_7 \, \bar{U}_{z,i,j,k} + V_8 \, \bar{U}_{z,i,j-1,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5\right.$$
$$\left. + V_7 + V_8\right)$$

2.
$V_1 = (iS + S/2 - x)(jS + 3S/2 - y)(kS + S/2 - y)$
$V_2 = (iS + S/2 - x)(y - S/2 - jS)(kS + S/2 - z)$
$V_3 = (iS + S/2 - x)(y - S/2 - jS)(z + S/2 - kS)$
$V_4 = (iS + S/2 - x)(jS + 3S/2 - y)(z + S/2 - kS)$
$V_5 = (x + S/2 - iS)(jS + 3S/2 - y)(kS + S/2 - z)$
$V_6 = (x + S/2 - iS)(y - S/2 - jS)(kS + S/2 - z)$
$V_7 = (x + S/2 - iS)(y - S/2 - jS)(z + S/2 - kS)$
$V_8 = (x + S/2 - iS)(jS + 3S/2 - y)(z + S/2 - kS)$

$$U_x^1 = \left(V_1 \, \bar{U}_{x,i-1,j,k-1} + V_2 \, \bar{U}_{x,i-1,j+1,k-1} + V_3 \, \bar{U}_{x,i-1,j+1,k}\right.$$
$$+ V_4 \, \bar{U}_{x,i-1,j,k} + V_5 \, \bar{U}_{x,i,j,k-1} + V_6 \, \bar{U}_{x,i,j+1,k-1}$$
$$\left. + V_7 \, \bar{U}_{x,i,j+1,k} + V_8 \, \bar{U}_{x,i,j,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5\right.$$
$$\left. + V_7 + V_8\right)$$

$$U_y^1 = \left(V_1 \, \bar{U}_{y,i-1,j,k-1} + V_2 \, \bar{U}_{y,i-1,j+1,k-1} + V_3 \, \bar{U}_{y,i-1,j+1,k}\right.$$
$$+ V_4 \, \bar{U}_{y,i-1,j,k} + V_5 \, \bar{U}_{y,i,j,k-1} + V_6 \, \bar{U}_{y,i,j+1,k-1}$$
$$\left. + V_7 \, \bar{U}_{y,i,j+1,k} + V_8 \, \bar{U}_{y,i,j,k}\right) \Big/ \left(V_1 + V_2 + V_3 + V_4 + V_5 + V_6\right.$$
$$\left. + V_7 + V_8\right)$$

$$\bar{U}_z^1 = \big(V_1 \bar{U}_{z,i-1,j,k} + V_2 \bar{U}_{z,i-1,j+1,k} + V_3 \bar{U}_{z,i-1,j+1,k+1}$$
$$+ V_4 \bar{U}_{z,i-1,j,k+1} + V_5 \bar{U}_{z,i,j,k} + V_6 \bar{U}_{z,i,j+1,k}$$
$$+ V_7 \bar{U}_{z,i,j+1,k+1} + V_8 \bar{U}_{z,i,j,k+1}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

4.
$$V_1 = (iS + S/2 - x)(jS + S/2 - y)(kS + 3S/2 - z)$$
$$V_2 = (iS + S/2 - x)(y + S/2 - jS)(kS + 3S/2 - z)$$
$$V_3 = (iS + S/2 - x)(y + S/2 - jS)(z - S/2 - kS)$$
$$V_4 = (iS + S/2 - x)(jS + S/2 - y)(z - S/2 - kS)$$
$$V_5 = (x + S/2 - iS)(jS + S/2 - y)(kS + 3S/2 - z)$$
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$$V_7 = (x + S/2 - iS)(y + S/2 - jS)(z - S/2 - kS)$$
$$V_8 = (x + S/2 - iS)(jS + S/2 - y)(z - S/2 - kS)$$

$$\bar{U}_x^1 = \big(V_1 \bar{U}_{x,i-1,j-1,k} + V_2 \bar{U}_{x,i-1,j,k} + V_3 \bar{U}_{x,i-1,j,k}$$
$$+ V_4 \bar{U}_{x,i-1,j-1,k+1} + V_5 \bar{U}_{x,i,j-1,k} + V_6 \bar{U}_{x,i,j,k}$$
$$+ V_7 \bar{U}_{x,i,j,k+1} + V_8 \bar{U}_{x,i,j-1,k+1}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

$$\bar{U}_y^1 = \big(V_1 \bar{U}_{y,i,j-1,k} + V_2 \bar{U}_{y,i-1,j-1,k} + V_3 \bar{U}_{y,i-1,j,k}$$
$$+ V_4 \bar{U}_{y,i-1,j-1,k+1} + V_5 \bar{U}_{y,i,j-1,k} + V_6 \bar{U}_{y,i,j,k}$$
$$+ V_7 \bar{U}_{y,i,j,k+1} + V_8 \bar{U}_{y,i,j-1,k+1}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

$$\bar{U}_z^1 = \big(V_1 \bar{U}_{z,i-1,j-1,k} + V_2 \bar{U}_{z,i-1,j,k} + V_3 \bar{U}_{z,i-1,j,k+1}$$
$$+ V_4 \bar{U}_{z,i-1,j-1,k+1} + V_5 \bar{U}_{z,i,j-1,k} + V_6 \bar{U}_{z,i,j,k}$$
$$+ V_7 \bar{U}_{z,i,j,k+1} + V_8 \bar{U}_{z,i,j-1,k+1}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

5.
$$V_1 = (iS + 3S/2 - x)(jS + S/2 - y)(kS + S/2 - z)$$
$$V_2 = (iS + 3S/2 - x)(y + S/2 - jS)(kS + S/2 - z)$$
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$$V_4 = (iS + 3S/2 - x)(jS + S/2 - y)(z + S/2 - kS)$$
$$V_5 = (x - S/2 - iS)(jS + S/2 - y)(kS + S/2 - z)$$
$$V_6 = (x - S/2 - iS)(y + S/2 - jS)(kS + S/2 - z)$$
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$$V_8 = (x - S/2 - iS)(jS + S/2 - y)(z + S/2 - kS)$$

$$\bar{U}_x^1 = \big(V_1 \bar{U}_{x,i,j-1,k-1} + V_2 \bar{U}_{x,i,j,k-1} + V_3 \bar{U}_{x,i,j,k}$$
$$+ V_4 \bar{U}_{x,i,j-1,k} + V_5 \bar{U}_{x,i+1,j-1,k-1} + V_6 \bar{U}_{x,i+1,j,k-1}$$
$$+ V_7 \bar{U}_{x,i+1,j,k} + V_8 \bar{U}_{x,i+1,j-1,k}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

$$\bar{U}_y^1 = \big(V_1 \bar{U}_{y,i,j-1,k-1} + V_2 \bar{U}_{y,i,j,k-1} + V_3 \bar{U}_{y,i,j,k}$$
$$+ V_4 \bar{U}_{y,i,j-1,k} + V_5 \bar{U}_{y,i+1,j-1,k-1} + V_6 \bar{U}_{y,i+1,j,k-1}$$
$$+ V_7 \bar{U}_{y,i+1,j,k} + V_8 \bar{U}_{y,i+1,j-1,k}\big)\big/\big(V_1 + V_2 + V_3 + V_4 + V_5$$
$$+ V_6 + V_7 + V_8\big)$$

$$\bar{v}^1_z = \left(v_1 \bar{U}_{z,i,j-1,k-1} + v_2 \bar{U}_{z,i,j,k-1} + v_3 \bar{U}_{z,i,j,k}\right.$$
$$+ v_4 \bar{U}_{x,i,j-1,k} + v_5 \bar{U}_{z,i+1,j-1,k-1} + v_6 \bar{U}_{z,i+1,j,k-1}$$
$$\left. + v_7 \bar{U}_{z,i+1,j-1,k} + v_8 \bar{U}_{z,i+1,j-1,k}\right)/\left(v_1 + v_2 + v_3 + v_4 + v_5\right.$$
$$\left. + v_6 + v_7 + v_8\right)$$

6.
$v_1 = (iS + 3S/2 - x)(jS + 3S/2 - y)(kS + S/2 - z)$
$v_2 = (iS + 3S/2 - x)(y - S/2 - jS)(kS + S/2 - z)$
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$v_8 = (x - S/2 - iS)(jS + 3S/2 - y)(z + S/2 - kS)$

$$\bar{v}^1_x = \left(v_1 \bar{U}_{x,i,j,k-1} + v_2 \bar{U}_{x,i,j+1,k-1} + v_3 \bar{U}_{x,i,j+1,k}\right.$$
$$+ v_4 \bar{U}_{x,i,j,k} + v_5 \bar{U}_{x,i+1,j,k-1} + v_6 \bar{U}_{x,i+1,j+1,k-1}$$
$$\left. + v_7 \bar{U}_{x,i+1,j+1,k} + v_8 \bar{U}_{x,i+1,j,k}\right)/\left(v_1 + v_2 + v_3 + v_4 + v_5\right.$$
$$\left. + v_6 + v_7 + v_8\right)$$

$$\bar{v}^1_y = \left(v_1 \bar{U}_{y,i,j,k-1} + v_2 \bar{U}_{y,i,j+1,k-1} + v_3 \bar{U}_{y,i,j+1,k}\right.$$
$$+ v_4 \bar{U}_{y,i,j,k} + v_5 \bar{U}_{y,i+1,j,k-1} + v_6 \bar{U}_{y,i+1,j+1,k-1}$$
$$\left. + v_7 \bar{U}_{y,i+1,j+1,k} + v_8 \bar{U}_{y,i+1,j,k}\right)/\left(v_1 + v_2 + v_3 + v_4 + v_5\right.$$
$$\left. + v_6 + v_7 + v_8\right)$$

$$\bar{v}^1_z = \left(v_1 \bar{U}_{z,i,j,k-1} + v_2 \bar{U}_{z,i,j+1,k-1} + v_3 \bar{U}_{z,i,j+1,k}\right.$$
$$+ v_4 \bar{U}_{x,i,j,k} + v_5 \bar{U}_{z,i+1,j,k-1} + v_6 \bar{U}_{z,i+1,j+1,k-1}$$
$$\left. + v_7 \bar{U}_{z,i+1,j+1,k} + v_8 \bar{U}_{z,i+1,j,k}\right)/\left(v_1 + v_2 + v_3 + v_4 + v_5\right.$$
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$v_1 = (iS + 3S/2 - x)(jS + 3S/2 - y)(kS + 3S/2 - z)$
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$$\bar{v}^1_x = \left(v_1 \bar{U}_{x,i,j,k} + v_2 \bar{U}_{x,i,j+1,k} + v_3 \bar{U}_{x,i,j+1,k+1}\right.$$
$$+ v_4 \bar{U}_{x,i,j,k+1} + v_5 \bar{U}_{x,i+1,j,k} + v_6 \bar{U}_{x,i+1,j+1,k}$$
$$\left. + v_7 \bar{U}_{x,i+1,j+1,k+1} + v_8 \bar{U}_{x,i+1,j,k+1}\right)/\left(v_1 + v_2 + v_3 + v_4\right.$$
$$\left. + v_5 + v_6 + v_7 + v_8\right)$$

$$\bar{v}^1_y = \left(v_1 \bar{U}_{y,i,j,k} + v_2 \bar{U}_{y,i,j+1,k} + v_3 \bar{U}_{y,i,j+1,k+1}\right.$$
$$+ v_4 \bar{U}_{y,i,j,k+1} + v_5 \bar{U}_{y,i+1,j,k} + v_6 \bar{U}_{y,i+1,j+1,k}$$
$$\left. + v_7 \bar{U}_{y,i+1,j+1,k+1} + v_8 \bar{U}_{y,i+1,j,k+1}\right)/\left(v_1 + v_2 + v_3 + v_4\right.$$
$$\left. + v_5 + v_6 + v_7 + v_8\right)$$

$$U_z^1 = \left(V_1 \bar{U}_{z,i,j,k} + V_2 \bar{U}_{z,i,j+1,k} + V_3 \bar{U}_{z,i,j+1,k+1}\right.$$
$$+ V_4 \bar{U}_{z,i,j,k+1} + V_5 \bar{U}_{z,i+1,j,k} + V_6 \bar{U}_{z,i+1,j+1,k}$$
$$+ V_7 \bar{U}_{z,i+1,j+1,k+1} + V_8 \bar{U}_{z,i+1,j,k+1}\left)\right/\left(V_1 + V_2 + V_3 + V_4\right.$$
$$\left.+ V_5 + V_6 + V_7 + V_8\right)$$

8.
$$V_1 = (iS + 3S/2 - x)(jS + S/2 - y)(kS + 3kS/2 - z)$$
$$V_2 = (iS + 3S/2 - x)(y + S/2 - jS)(kS + 3S/2 - z)$$
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$$V_6 = (x - S/2 - jS)(y + S/2 - jS)(kS + 3kS/3 - z)$$
$$V_7 = (x - S/2 - jS)(y + S/2 - jS)(z - S/2 - kS)$$
$$V_8 = (x - S/2 - jS)(jS + 3/2 - y)(z - S/2 - kS)$$

$$U_x^1 = \left(V_1 \bar{U}_{x,i,j-1,k} + V_2 \bar{U}_{x,i,j,k} + V_3 \bar{U}_{x,i,j,k+1}\right.$$
$$+ V_4 \bar{U}_{x,i,j-1,k+1} + V_5 \bar{U}_{x,i+1,j-1,k} + V_6 \bar{U}_{x,i+1,j,k}$$
$$+ V_7 \bar{U}_{x,i+1,j,k+1} + V_8 \bar{U}_{x,i+1,j-1,k+1}\left)\right/\left(V_1 + V_2 + V_3 + V_4\right.$$
$$\left.+ V_5 + V_6 + V_7 + V_8\right)$$

$$U_y^1 = \left(V_1 \bar{U}_{y,i,j-1,k} + V_2 \bar{U}_{y,i,j,k} + V_3 \bar{U}_{y,i,j,k+1}\right.$$
$$+ V_4 \bar{U}_{y,i,j-1,k+1} + V_5 \bar{U}_{y,i+1,j-1,k} + V_6 \bar{U}_{y,i+1,j,k}$$
$$+ V_7 \bar{U}_{y,i+1,j,k+1} + V_8 \bar{U}_{y,i+1,j-1,k+1}\left)\right/\left(V_1 + V_2 + V_3 + V_4 + V_5\right.$$
$$\left.+ V_6 + V_7 + V_8\right)$$

The new position of the particle is calculated from these velocities.

$$x' = x + U_x^1 \, \Delta t$$
$$y' = y + U_y^1 \, \Delta t$$
$$z' = z + U_z^1 \, \Delta t$$

If a particle moves across a boundary out of the range of calculation, it is removed from the calculation by setting its mass to zero. The appropriate fractions of energy and momenta are subtracted from the cell it left.

If a particle (of mass m) moves from one cell (i,j,k) to another (l,m,n), the cell quantities are adjusted as follows.

$$M'_{i,j,k} = M_{i,j,k} - m$$
$$M'_{l,m,n} = M_{l,m,n} + m$$

$$\bar{X}'_{x,i,j,k} = \bar{X}_{x,i,j,k} - m \bar{U}_{x,i,j,k}$$
$$\bar{X}'_{y,i,j,k} = \bar{X}_{y,i,j,k} - m \bar{U}_{y,i,j,k}$$
$$\bar{X}'_{z,i,j,k} = \bar{X}_{z,i,j,k} - m \bar{U}_{z,i,j,k}$$

$$\bar{X}'_{x,l,m,n} = \bar{X}_{x,l,m,n} + m \bar{U}_{x,i,j,k}$$
$$\bar{X}'_{y,l,m,n} = \bar{X}_{y,l,m,n} + m \bar{U}_{y,i,j,k}$$
$$\bar{X}'_{z,l,m,n} = \bar{X}_{z,l,m,n} + m \bar{U}_{z,i,j,k}$$

PHASE III

$$E'_{i,j,k} = E_{i,j,k} - \frac{m}{m} I_{i,j,k} B_{i,j,k}$$

$$E'_{\ell,m,n} = E_{\ell,n,n} + \frac{m}{M_{i,j,k}} B_{i,j,k}$$

$$V'_{\ell,m,n} = \frac{M_{\ell,m,n} W_{\ell,m,n} + m W_{i,j,k}}{M_{\ell,m,n} + m}$$

A. The velocities and internal energy are calculated from the momenta and total energy.

$$U_{x,i,j,k} = \frac{X_{x,i,j,k}}{M_{i,j,k}}$$

$$U_{y,i,j,k} = \frac{X_{y,i,j,k}}{M_{i,j,k}}$$

$$U_{z,i,j,k} = \frac{X_{z,i,j,k}}{M_{i,j,k}}$$

$$I_{i,j,k} = \frac{E_{i,j,k}}{M_{i,j,k}} - \frac{1}{2}\left(U^2_{x,i,j,k} + U^2_{y,i,j,k} + U^2_{z,i,j,k}\right)$$

B. Chemical reaction is performed according to the Arrhenius rate law[2].

$$W'_{i,j,k} = W_{i,j,k}\left[1 - (z)(\Delta t) e^{-E^*/R\,T_{i,j,k}}\right]$$

C. The equation of state used is the HOM equation of state[2,3]. Given the specific volume, internal energy, and mass fraction of a cell, HOM calculates the temperature and pressure. For specific volumes less than the initial value, the pressure and temperature are set to their initial

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values. If the mass of a cell is zero, the pressure and temperature are also set to zero.

D. The total time is increased by Δt, and the calculation begins with Phase I.

THE NOMENCLATURE

Quantities pertaining to cell ijk

$E_{i,j,k}$	total energy
$I_{i,j,k}$	internal energy
$M_{i,j,k}$	mass
$P_{i,j,k}$	pressure
$P^{\ell}_{i,j,k}$	pressure on face ℓ
$G^{\ell}_{i,j,k}$	viscosity pressure on face ℓ
S	length of cell side (2×10^{-3} cm)
$T_{i,j,k}$	temperature
$U_{x,i,j,k}$	x velocity
$U_{y,i,j,k}$	y velocity
$U_{z,i,j,k}$	z velocity
$W_{i,j,k}$	mass fraction of undecomposed explosive
$X_{x,i,j,k}$	momentum in x direction
$X_{y,i,j,k}$	momentum in y direction
$X_{z,i,j,k}$	momentum in z direction

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STEREO PLOTTING

We shall describe a technique for stereo plotting a set of points in three dimensions. This method was developed by K. Crandall and R. Lewis of the Los Alamos Scientific Laboratory.

From the direction of sight, three unit vectors are determined.

$\bar{e}_1$ in the direction of the viewer's line of sight

$\bar{e}_2$ points from the right eye to the left eye

$\bar{e}_3 = \bar{e}_1 \times \bar{e}_2$

A plane is then constructed perpendicular to $\bar{e}_1$ through the point with the minimum scalar product with $\bar{e}_1$; i.e., if the plane is moved closer to the viewer, all the points are beyond it, and if it is moved away, there are points between it and the viewer. All the points are projected onto this plane to determine the size square which will contain all the points in the three-dimensional views. From this window size and the characteristics of the stereo viewer, one determines the distance, d, that the eyes should be from this plane. The position of the eyes is then found by going a distance d in the $-\bar{e}_1$ direction from the center of the window and then a short distance along $\bar{e}_2$ and $-\bar{e}_2$ to separate the two eyes. The window size is then divided by d to get the window size at a unit distance from the eyes. A plane is constructed at this point perpendicular to $\bar{e}_1$ with a coordinate system (x', y'); the x' axis in the $-\bar{e}_2$ direction and the y' axis in the $\bar{e}_3$ direction.

The stereo pictures are produced by taking one eye at a time, connecting it by a straight line to each point, finding the intersection with the plane a unit distance from the eyes, and determining the (x', y') coordinates of the point of intersection. These coordinates are then used to plot the point on the SC-4020.

NOMENCLATURE (continued)

Quantities pertaining to each particle

m	mass
U_x^i	x velocity
U_y^i	y velocity
U_z^i	z velocity
x	x coordinate
y	y coordinate
z	z coordinate
Δt	time increment (5 x 10^{-4} sec)
ρ	density

The mathematical techniques are as follows:

Given $\vec{e}_1 = (e_{1x}, e_{1y}, e_{1z})$ and a set of points $\{\vec{r}_k\}$ in three dimensions, define

$$\vec{e}_2 = \frac{1}{\sqrt{e_{1x}^2 + e_{1y}^2}} (e_{1y}, -e_{1x}, 0)$$

$$\vec{e}_3 = \vec{e}_1 \times \vec{e}_2 . \qquad (a)$$

If e_{3z} is negative, replace $\vec{e}_2$ by $-\vec{e}_2$ and $\vec{e}_3$ by $-\vec{e}_3$. This assures that $\vec{e}_2$ points from the right eye to the left and $\vec{e}_3$ points upward.

The position of the plane of projection is determined by finding the point $\vec{r}_m$ which minimizes $\vec{r}_k \cdot \vec{e}_1$ (b). One then projects each of the points $\vec{r}_k$ into this plane and determines their (x'_k, y'_k) coordinates.
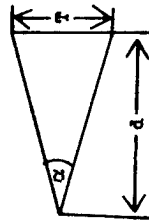
$$x'_k = -\vec{e}_2 \cdot \left([(\vec{r}_m - \vec{r}_k) \cdot \vec{e}_1]\vec{e}_1 + \vec{r}_k \right) \qquad (c)$$

$$y'_k = \vec{e}_3 \cdot \left([(\vec{r}_m - \vec{r}_k) \cdot \vec{e}_1]\vec{e}_1 + \vec{r}_k \right) \qquad (d)$$

Let $\bar{x} = \max_k \{x'_k\}$, $\bar{y} = \max_k \{y'_k\}$

$\hat{x} = \min_k \{x'_k\}$ and $\hat{y} = \min_k \{y'_k\}$.

For a given stereo viewer there is an angular limit, α, to the field of vision. The distance, d, of the eyes from the plane of projection is determined by T, the width of the window, and α. The half-

window width at a unit distance from the eyes $w = \frac{T}{d}$ is a constant for each viewer. The eyes are separated by a distance $\frac{2sT}{1+s}$ where the value of s is again dependent upon the stereo viewer. The distance, d, the eyes must be from the plane in order to see everything in the x' direction is $d \geq \frac{(\bar{x} - \hat{x})(1+s)}{w}$. To see everything in the y direction, $d \geq \frac{(\bar{y} - \hat{y})}{w}$. The larger of these two distances is taken as the distance of the eyes from the center of the window $\vec{e}_1$. The size, T, of a side of the square window is then either $(1+s)(\bar{x} - \hat{x})$ or $(\bar{y} - \hat{y})$.

The vector to the center of the projection is

$$\vec{c} = (\vec{r}_m \cdot \vec{e}_1)\vec{e}_1 - \frac{(\bar{x} + \hat{x})}{2}\vec{e}_2 + \frac{(\bar{y} + \hat{y})}{2}\vec{e}_3 , \qquad (e)$$

the vector to the right eye is

$$\vec{r}_r = \vec{c} - d\vec{e}_1 - \frac{Ts}{1+s}\vec{e}_2 , \qquad (f)$$

and the one to the left is

$$\vec{r}_l = \vec{c} - d\vec{e}_1 + \frac{Ts}{1+s}\vec{e}_2 . \qquad (g)$$

The two pictures are then made on the SC-4020, plotting the view for the left eye first. The coordinates of the point of intersection of a line from an eye to a point $\vec{r}_k$ and a plane a unit distance away from the eyes are

$$x_k = \left(\frac{\vec{r}_k - \vec{r}}{(\vec{r}_k - \vec{r}) \cdot \vec{e}_1} - \vec{e}_1 \right) \cdot \vec{e}_2 , \qquad (h)$$

and

$$y_k = \left(\frac{\vec{r}_k - \vec{r}}{(\vec{r}_k - \vec{r}) \cdot \vec{e}_1} - \vec{e}_1 \right) \cdot \vec{e}_3 , \qquad (i)$$

where $\vec{r}$ is a vector to one of the eyes. These coordinates (x_k, y_k) are then plotted using the PLTLN routine on SKETCH with grid boundaries of $-w$ to w in both x and y directions.

For Figures 5 and 6 we used the following parameters.

$w = 0.3$
$s = 0.25$
$\vec{e}_1 = (0,\ 0.96593,\ -0.25882) = (0,\ \cos 15°,\ -\sin 15°)$
$\vec{e}_2 = (-1,\ 0,\ 0)$
$\vec{e}_3 = (0,\ 0.25882,\ 0.96593)$.

The coding formulas for the equations above designated by letters are as follows.

(a) The components of $\vec{e}_3$ are

$e_{3x} = e_{1y}e_{2z} - e_{1z}e_{2y}$

$e_{3y} = e_{1z}e_{2x} - e_{1x}e_{2z}$

$e_{3z} = e_{1x}e_{2y} - e_{1y}e_{2x}$.

(b) $r_{kx}e_{1x} + r_{ky}e_{1y} + r_{kz}e_{1z} = r_{kx}e_{1x} + r_{ky}e_{1y}$
$+\ r_{kz}e_{1z}$ for all k.

(c) and (d) Since $\vec{e}_2 \cdot \vec{e}_1 = \vec{e}_3 \cdot \vec{e}_1 = 0$,

$x'_k = -e_{3x}r_{kx} - e_{2y}r_{ky} - e_{2z}r_{kz}$

$y'_k = e_{3x}r_{kx} + e_{3y}r_{ky} + e_{3z}r_{kz}$.

(e) $c_x = (r_{mx}e_{1x} + r_{my}e_{1y} + r_{mz}e_{1z})e_{1x} - \dfrac{(\bar{x}+\hat{x})}{2}e_{3x}$
$+\ \dfrac{(\bar{y}+\hat{y})}{2}e_{3x}$

$c_y = (r_{mx}e_{1x} + r_{my}e_{1y} + r_{mz}e_{1z})e_{1y} - \dfrac{(\bar{x}+\hat{x})}{2}e_{2y}$
$+\ \dfrac{(\bar{y}+\hat{y})}{2}e_{3y}$

$c_z = (r_{mx}e_{1x} + r_{my}e_{1y} + r_{mz}e_{1z})e_{1z} - \dfrac{(\bar{x}+\hat{x})}{2}e_{2z}$
$+\ \dfrac{(\bar{y}+\hat{y})}{2}e_{3z}$.

(f) $Y_{rx} = c_x - de_{1x} - \dfrac{rs}{1+s}e_{2x}$

$Y_{ry} = c_y - de_{1y} - \dfrac{rs}{1+s}e_{2y}$

$Y_{rz} = c_z - de_{1z} - \dfrac{rs}{1+s}e_{2z}$.

(g) $Y_{sx} = c_x - de_{1x} + \dfrac{rs}{1+s}e_{2x}$

$Y_{sy} = c_y - de_{1y} + \dfrac{rs}{1+s}e_{2y}$

$Y_{sz} = c_z - de_{1z} + \dfrac{rs}{1+s}e_{2z}$.

(h) and (i) Since $\vec{e}_1 \cdot \vec{e}_2 = \vec{e}_1 \cdot \vec{e}_3 = 0$,

$$x_k = \frac{(r_{kx} - Y_x)e_{2x} + (r_{ky} - Y_y)e_{2y} + (r_{kz} - Y_z)e_{2z}}{(r_{kx} - Y_x)e_{1x} + (r_{ky} - Y_y)e_{1y} + (r_{kz} - Y_z)e_{1z}}$$

$$y_k = \frac{(r_{kx} - Y_x)e_{3x} + (r_{ky} - Y_y)e_{3y} + (r_{kz} - Y_z)e_{3z}}{(r_{kx} - Y_x)e_{1x} + (r_{ky} - Y_y)e_{1y} + (r_{kz} - Y_z)e_{1z}}$$.

END

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